

Square lattice self-avoiding walks and biased differential approximants

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Abstract. The model of self-avoiding lattice walks and the asymptotic analysis of power-series have been two of the major research themes of Tony Guttmann. In this paper we bring the two together and perform a new analysis of the generating functions for the number of square lattice self-avoiding walks and some of their metric properties such as the mean-square end-to-end distance. The critical point x_c for self-avoiding walks is known to a high degree of accuracy and we utilise this knowledge to undertake a new numerical analysis of the series using biased differential approximants. The new method is major advance in asymptotic power-series analysis in that it allows us to bias differential approximants to have a singularity of order q at x_c . When biasing at x_c with $q \geq 2$ the analysis yields a very accurate estimate for the critical exponent $\gamma = 1.3437500(3)$ thus confirming the conjectured exact value $\gamma = 43/32$ to 8 significant digits and removing a long-standing minor discrepancy between exact and numerical results. The analysis of the mean-square end-to-end distance yields $\nu = 0.7500002(4)$ thus confirming the exact value $\nu = 3/4$ to 7 significant digits.

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1. Introduction

In Tony Guttmann's long and distinguished career the model of self-avoiding walks and how to analyse its behaviour has been a mainstay. Since the early years [1] to the present day [2] Tony has published more than 130 papers on self-avoiding walks, polygons and closely related models. At the same time Tony has made many important and seminal contributions to the development of new methods for asymptotic analysis of power-series, chief amongst these the method of differential approximants [3, 4].

A *n-step self-avoiding walk* (SAW) ω on a regular lattice is a sequence of *distinct* vertices $\omega_0, \omega_1, \dots, \omega_n$ such that each vertex is a nearest neighbour of its predecessor. SAW are considered distinct up to translations of the starting point ω_0 . If ω_0 and ω_n are nearest-neighbours we can form a closed polygon *n-step self-avoiding polygon*

(SAP) by adding an edge between the two end-points. The fundamental problem is the calculation of the number of SAW, c_n , with n steps. As most interesting combinatorial problems, SAW have exponential growth. The generating function for SAW (and SAP) is believed to have algebraic singularities, though in most cases this has not been proved. That is to say, the generating function is believed to behave as

$$F(x) = \sum_{n=0}^{\infty} c_n x^n \sim A(1 - x/x_c)^{-\gamma} \text{ as } x \rightarrow x_c^-. \quad (1)$$

Here A is referred to as the *critical amplitude*, x_c as the *critical point*, and γ as the *critical exponent*. The value of $\gamma = 43/32$ is known exactly [5, 6], though it remains to be proved rigorously. Besides the physical singularity there is another singularity at $x = x_- = -x_c$ [7, 8] which has a critical exponent consistent with the exact value $1/2$.

Before one can say much about the behaviour of self-avoiding walks one must have something to work with so Tony has pushed hard for major strides to be made in the development of new and improved algorithms [9] for counting self-avoiding walks. And given that these counting problems are inherently of exponential time complexity Tony and his co-workers have always been eager to make use of the latest progress in computing technology including being early adapters of massively parallel computations [10]. The data for self-avoiding walks has been used to obtain very accurate numerical tests of analytic predictions originating from scaling theory, conformal field theory, stochastic Loewner evolution, etc. [8, 11, 12]. Besides the already mentioned method of differential approximants the intricacies of the asymptotic behaviour of various walk problem has spurred Tony's development of new methods for asymptotic analysis of power-series [13, 14, 15]. The full self-avoiding walk model is well known to be a very tough problem with no immediate prospect of an exact solution. In fact Tony used SAW as a prime testing ground for ideas on how to determine whether or not a given model is solvable [16, 17]. Tony has been an avid advocate for the utility of studying simpler exactly solvable problem both as an important and interesting pursuit in its own right and as a means of gaining further insight into the original harder problem. This work has resulted in many exact solutions to simpler (often directed) walk problems [18, 19, 20, 21] including one of the very few exact solutions for a 3D lattice model [22, 23]. One particular result vividly illustrates why the study of simple solvable lattice models can contribute in a major way to our understanding of more complicated problem. In a series of papers Tony and co-workers demonstrated that the study of the simple model of staircase polygons could lead one to conjecture the area-perimeter scaling function for self-avoiding polygons [24, 25, 26]. Finally, we mention that Tony has been involved in many research projects which have used self-avoiding walk to model many aspects of polymer physics and chemistry including steric stabilisation [27], modelling of vesicles [28], polymer collapse and interacting walks [29, 30, 31, 32], polymer adsorption and desorption from a surface [14, 33], force-induced polymer unfolding [34, 35] and desorption [36].

So one can safely say that self-avoiding walks have been very good to Tony and

that Tony has been exceptionally good for our understanding of the self-avoiding walk problem and its many and varied uses in the modelling of physical, chemical and biological systems.

In this paper we bring together two of Tony's favourites and perform a new numerical analysis of the generating functions for the number of square lattice self-avoiding walks and some of their metric properties. From the numerical analysis (using differential approximants) of the generating function for square lattice self-avoiding polygons we have obtained very accurate estimates for the critical point $x_c^2 = 0.143680629269(2)\ddagger$ and critical exponent $\alpha = 0.500000015(20)$ [37]. However, for square lattice SAW there is an annoying (at least to the author) minor discrepancy between the above prediction for the exact values of the critical exponents and the estimates from series analysis where our best estimate using standard differential approximants $\gamma = 1.343745(3)$ is agonisingly close to the exact value $\gamma = 43/32 = 1.34375$. Now no one would seriously take this minor discrepancy as an indication that the conjectured exact value isn't correct, rather it is a 'deficiency' in the numerical analysis. In this paper we show how this discrepancy can be eliminated by the use of *biased differential approximants*. With this new analysis we can confirm the value of the critical exponent to at least 8 significant digits. We also carry out a biased analysis of the generating functions for the metric properties (end-to-end distance, monomer-to-end distance and radius of gyration) that confirms to 7 digits accuracy that the size exponent $\nu = 3/4$.

2. Biased differential approximants

From the known exact solutions to various directed walk and polygon problems it is clear that the generating functions are often algebraic or given by the solution of simple linear ordinary differential equations [18, 19, 20, 38]. This observation (originally made in the context of the Ising model) forms the nucleus of the method of *differential approximants*. The basic idea is to approximate the function $F(x)$ by solutions to differential equations with polynomial coefficients. The singular behaviour of such ODEs is a well known classical mathematics problem (see e.g. [39, 40]) and the singular points and exponents are easily calculated. Even if the function *globally* is not a solution of a such a linear ODE (as is the case for SAW) one hopes that *locally* in the vicinity of the (physical) critical points the generating function can still be well approximated by a solution to a linear ODE.

A K th-order differential approximant (DA) to a function $F(x)$ is formed by representing the function by a K th-order ODE (possibly inhomogenous) with polynomial coefficients such that

$$P(x) + \sum_{k=0}^K Q_k(x) \left(x \frac{d}{dx} \right)^k F(x) = O(x^{N+1}). \quad (2)$$

\ddagger The critical point for square lattice SAP is at x_c^2 because every polygon has even length.

Here $Q_k(x)$ and $P(x)$ are polynomials of degree N_k and L , respectively, and

$$N = L + 1 + \sum_{k=0}^K (N_k + 1)$$

is the number of unknown coefficients. Determining these coefficients such that (2) is satisfied then amount to solving a system of linear equations. So we have that (one) of the formal power-series solutions to the ODE agrees with the series expansion of the (generally unknown) function $F(x)$ up to the first N coefficients.

From the theory of ODEs, the singularities of $F(x)$ are approximated by the roots, x_i ($i = 1, \dots, N_K$), of $Q_K(x)$, and the associated critical exponents λ_i are estimated from the indicial equation. The physical critical point x_c is generally the singularity on the positive real axis closest to the origin. When the root at x_i has order q we can find the associated exponents by forming the indicial polynomial

$$P_I(z) = \sum_{m=0}^q \frac{x_i^m}{m!} \cdot Q_{K-q+m}^{(m)}(x_i) \cdot [z]_m, \quad (3)$$

where $[z]_m = z(z-1)\cdots(z-m+1)$, $[z]_0 = 1$. Then if z_j , ($j = 1, \dots, q$) are the roots of $P_I(z)$ the associated critical exponents have values $\lambda_{i,j} = K - q + z_j$. If there is only a single root at x_i this is just

$$\lambda_i = K - 1 - \frac{Q_{K-1}(x_i)}{x_i Q'_K(x_i)}. \quad (4)$$

By varying the degrees of the polynomials one can generate a large set of differential approximants to $F(x)$. Each approximant yields values for x_c and γ and by averaging over several (often hundreds) of these one can calculate estimates for these critical parameters (see [41, Ch 8] for more details). We denote individual approximants by the notation $[N_K, N_{K-1}, \dots, N_0; L]_{\S}$. In general one focuses on so-called close to diagonal approximants where N_k , $k < K$, differ from N_K by a small amount and one may typically use the restriction $|N_K - N_k| \leq 1$ or 2.

If the critical point x_c is known exactly (or very accurately) one may try to obtain improved numerical estimates for the exponents by forcing the differential equation (2) to have a singular point at x_c , that is one may look at *biased differential approximants*. We have developed a new method in which we form biased approximants by multiplying the derivatives in (2) by appropriate “biasing polynomials”. This allows us to bias in such a manner that the singularity at x_c is of order $q \leq K$. Let

$$F_k(x) = \left(x \frac{d}{dx}\right)^k F(x) \quad \text{and} \quad G_k(x) = (1 - x/x_c)^{q_k} F_k(x), \quad (5)$$

where $q_k = \max(q + k - K, 0)$. With this definition we have that $G_k = (1 - x/x_c)^q F_k(x)$, while subsequent lower order derivatives have “biasing polynomials” of degree decreasing

\S Note that in the $L = 0$ case $P(x) = 0$ rather than a non-zero constant.

in steps of 1 (until 0). This choice corresponds to assuming that the singularity is regular [40]. Then we form biased differential approximants (BDA) such that

$$P(x) + \sum_{k=0}^K \widehat{Q}_k(x) G_k(x) = O(x^{N+1}). \quad (6)$$

One can readily generalise this to include further singularities at x_i with the order of each given by q_i and the singularity at x_i need not be given by a monomial as above but could in general be given by the root of a polynomial $p(x)$ with $p(x)$ used as (a factor in) the “biasing polynomial”. For biased approximants $[N_K, N_{K-1}, \dots, N_0; L]$ still denotes a case in which the degree of the polynomial multiplying the k 'th derivative have degree N_k such that the degrees of $\widehat{Q}_k(x) = N_k - q_k$ and the number of unknown coefficients is now

$$N = L + 1 + \sum_{k=0}^K (N_k - q_k + 1).$$

3. Analysis and Results

The critical point for square lattice self-avoiding walks is not known exactly but has been estimated to a high level of accuracy. Series analysis of the self-avoiding polygon series [37] yielded the estimate $x_c = 0.379052277752(3)$ which recently has been improved by Guttmann, Jacobsen and Scullard [42] to $x_c = 0.3790522777552(3)$ and henceforth we shall adopt the value $x_c = 0.3790522777552$. As mentioned in the introduction numerical estimates for the SAW critical exponent γ from un-biased DAs are close to the exact value but not quite on target. This means that square lattice SAW should be the perfect model on which to test the efficacy of our new approach to biased differential approximants. The number of square lattice SAW has been calculated up to length $n = 79$ and the generating functions for the metric properties of SAW up to length $n = 71$ [43].

3.1. The SAW generating function

First we take a look at results obtained from 3rd order differential approximants both un-biased ($q = 0$) and biased with the order of the root at x_c being $q = 1, 2$ and 3 . We generate lots of homogenous and inhomogenous ($L = 2, 4, 6, 8, 10$) approximants by varying N_3 from 8 to 20 and for each value of N_3 we generate all approximants with $|N_3 - N_k| \leq 1, k = 0, 1, 2$ (this amounts to more than 1600 approximants for each case). The smallest degree approximants thus utilise around 40 terms and the highest degree all 79 terms in the SAW generating function. In figure 1 we plot the resulting estimates of γ as a function of N . The panel for $q = 0$ (un-biased case) vividly illustrates the frustration the author has had in analysing this series. As can be seen the estimates exhibit a slow systematic drift as N is increasing and ever so slowly they creep towards the exact value (though one might question whether they would ever get there). Now for $q = 1$ the estimates get much closer to the exact value (note the different scale on

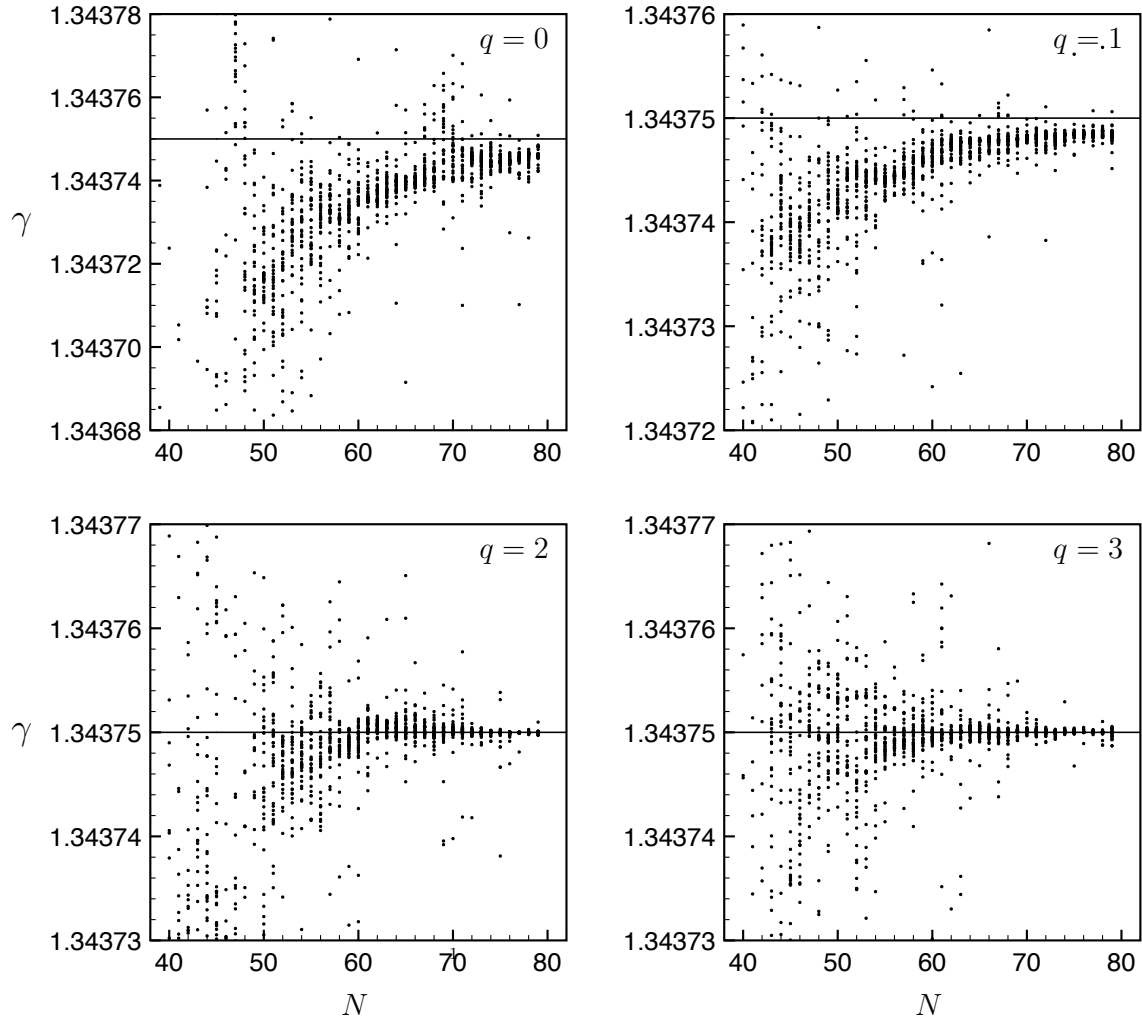


Figure 1. Estimates of the critical exponent γ of square lattice SAW as obtained from 3rd order differential approximants. The exponent estimates are plotted versus the number of terms N used to form the DA. The panels show the results from unbiased DAs ($q = 0$) and DAs biased to have a singularity at $x_c = 0.3790522777552$ with the order of the root changing from $q = 1$ to 3.

the y -axis), but again the approach is slow and not quite there yet. The explanation for this is fairly simple. If one looks at some individual approximants and calculate the roots of $\hat{Q}_K(x)$ one finds a root that is very close to x_c indicating that the series feels the presence of a confluent singularity at x_c and that $q = 1$ is therefore not sufficient biasing to pin down the critical behaviour. So we look to the $q = 2$ and 3 cases and now we find a very good convergence of the estimates to the exact value. For large value of N there is no discernible difference between the two cases but for low values of N the $q = 3$ biased approximants are superior. We also note that $\hat{Q}_K(x)$ does not have a root close to x_c when $q \geq 2$ thus confirming that the biasing has successfully accounted for the critical behaviour.

As noted in the introduction the SAW generating function also has a singularity

Table 1. Estimates for the critical exponent γ obtained from K th order biased differential approximants. We vary the order of the root at x_c from $q = 1$ to K and that at $-x_c$ from $r = 0$ to $\min(q, 2)$.

$[K, q, r]$	γ	$[K, q, r]$	γ	$[K, q, r]$	γ
[2, 1, 0]	1.34374784(48)	[2, 1, 1]	1.34374779(50)		
[3, 1, 0]	1.34374830(25)	[3, 1, 1]	1.34374831(25)		
[4, 1, 0]	1.34374838(39)	[4, 1, 1]	1.34374832(39)		
[2, 2, 0]	1.34375009(15)	[2, 2, 1]	1.34375008(13)	[2, 2, 2]	1.34375008(13)
[3, 2, 0]	1.34375003(10)	[3, 2, 1]	1.34375004(12)	[3, 2, 2]	1.34375002(10)
[4, 2, 0]	1.34374997(15)	[4, 2, 1]	1.34375000(15)	[4, 2, 2]	1.34375000(14)
[3, 3, 0]	1.343750024(80)	[3, 3, 1]	1.343750025(72)	[3, 3, 2]	1.343750041(62)
[4, 3, 0]	1.34375003(13)	[4, 3, 1]	1.34375004(13)	[4, 3, 2]	1.34375004(14)
[4, 4, 0]	1.343750059(62)	[4, 4, 1]	1.343750057(84)	[4, 4, 2]	1.343750071(92)

on the negative real axis at $x = x_- = -x_c$ with critical exponent of $1/2$. We can easily bias the approximants to include this singularity as well. In forming the biased approximants (6) we simply modify the biasing done in (5) to include the terms $(1 + x/x_c)^{r_k}$ in $G_k(x)$, where $r_k = \max(r + k - K, 0)$. This corresponds to biasing with a root of order r at $-x_c$. One can naturally vary q and r independently. As per above we calculate a large set of biased approximants in the cases of $K = 2, 3$, and 4 and $q = 1$ to K . To obtain estimates for γ we extract the relevant critical exponent (recall there are q critical exponents at x_c in a biased approximant) and we only results from approximants with $N \geq 70$. The exponents are sorted, next we remove or “clip” the bottom and top 10% of this data^{||} and calculate the mean and standard deviation of the remaining exponents. The results are displayed in table 1 where we list the estimates obtained from the mean. In parenthesis we show the standard deviation as an ‘error’ estimate on the last two digit. So the result 1.34375008(13) says that the mean was 1.34375008 and the standard deviation was 0.00000013. Note that we are *not* claiming that the standard deviation is the true error estimate. To be on the safe side one should use an error bound of at least two to three times the error estimate and one should always check as done here by plotting exponent estimates versus N that there is no systematic drift in the exponent estimates. The results in table 1 are in complete accordance with the observation from above that for $q \geq 2$ the biased estimates are spot-on the exact value. We are in fact confident in saying that the value of γ can be confirmed to at least significant 8 digits. We note that there is no improvement to the estimates from $r = 0$ to $r = 1$ or 2 , so biasing the approximants at $-x_c$ makes no difference at all to the estimates for γ . Finally, it is worth mentioning that changing the ‘clipping’ to say 5% or 20% has next to no effect of the mean but does change the standard deviation somewhat. In conclusion we claim that our new biased differential

^{||} This procedure will automatically eliminate any spurious outliers some of which will always be present when so many approximants are generated.

Table 2. Estimates for the critical exponent γ_- at $x = -x_c$ obtained from 3rd order biased differential approximants. We vary the order of the root at x_c from $q = 0$ to 3 and that at $-x_c$ from $r = 1$ to 3.

$[K, q, r]$	γ_-	$[K, q, r]$	γ_-	$[K, q, r]$	γ_-
$[3, 0, 1]$	0.5000014(13)	$[3, 0, 2]$	0.5000011(21)	$[3, 0, 3]$	0.5000011(20)
$[3, 1, 1]$	0.5000014(12)	$[3, 1, 2]$	0.5000009(29)	$[3, 1, 3]$	0.5000014(24)
$[3, 2, 1]$	0.5000013(10)	$[3, 2, 2]$	0.5000008(20)	$[3, 2, 3]$	0.5000008(26)
$[3, 3, 1]$	0.5000012(12)	$[3, 3, 2]$	0.5000015(27)	$[3, 3, 3]$	0.5000010(23)

approximant method yields a conservative estimate $\gamma = 1.3437500(3)$.

Next we perform a similar analysis but for the exponent γ_- at the singularity $x_- = -x_c$. The results for $K = 3$ are listed in table 2. As can be seen the exponent value $\gamma_- = 1/2$ can be confirmed to at least 5 significant digits and there is no change in the estimates as one changes r and q (even the $q = 0$ case gives similar estimates). We note that an un-biased analysis gives $\gamma_- = 0.500015(15)$, that is, an order of magnitude less accurate.

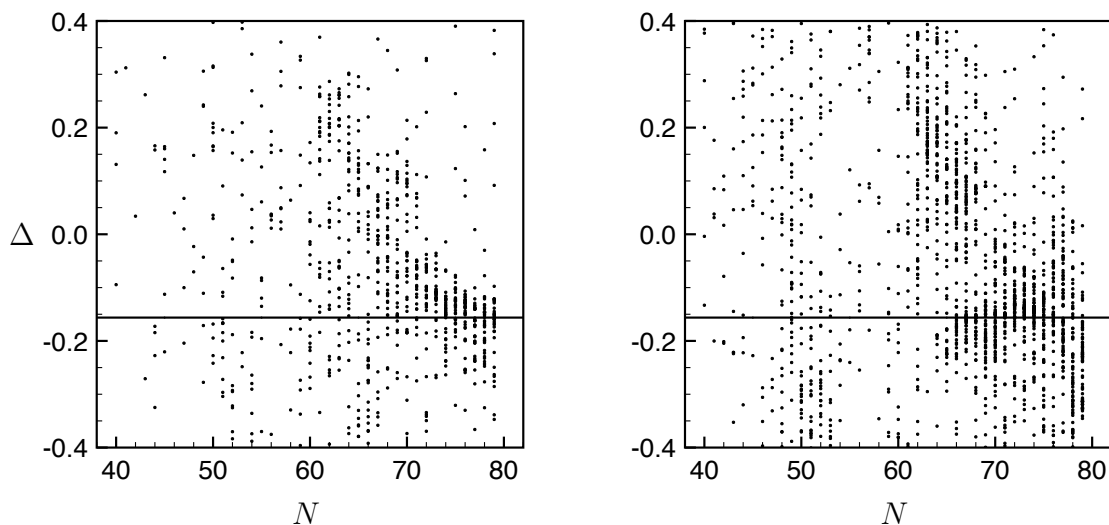


Figure 2. Estimates of the sub-dominant critical exponent for square lattice SAW. The left panel is for $K = 3, q = 2$ and the right panel $K = 4, q = 2$. The straight line corresponds to the value $\Delta = 3/2$ for the leading non-analytic correction to scaling exponent.

Finally, we address the question of estimating the sub-dominant exponents γ_s . The leading correction-to-scaling exponent is expected to have the exact value $\Delta = 3/2$ [5, 6]. In [11] the correction-to-scaling exponents for SAW was estimated numerically and a detailed and careful analysis unequivocally confirmed that $\Delta = 3/2$ is correct. But can we confirm this value from a biased differential approximant analysis? For $q \geq 2$ there are q exponent values at x_c and one might hope that of these (just the second exponent

in the case $q = 2$) will equal $\gamma_s = -\gamma + \Delta = 5/32$. Figure 2 shows the estimates for $-\gamma_s$ plotted versus N in the cases of $q = 2$ and $K = 3$ and 4. The straight line is the value $\gamma - \Delta = -5/32$ and as can be seen the estimates are certainly consistent with this value for large enough N . Unfortunately that is all one can say. So biasing does not lead to an accurate estimate for Δ . This does not change for higher values of q where similar plots can be made (the third and fourth exponents are of no use whatsoever).

3.2. Metric properties

Finally we analyse the generating functions for three metric properties. Firstly $\mathcal{R}_e(x)$ the mean-square end-to-end distance of an n step SAW, secondly $\mathcal{R}_m(x)$ the mean-square distance of a monomer (or vertex) from the end-points and thirdly $\mathcal{R}_g(x)$ the mean-square radius of gyration of the monomers of the SAW. Precise definitions of the relevant quantities can be found in say [11]. Suffice to that these functions are expected to have the critical behaviour

$$\mathcal{R}_e(x) = \sum_n c_n \langle R_e^2 \rangle_n x^n \quad \propto \quad (1 - x/x_c)^{-(\gamma+2\nu)}, \quad (7)$$

$$\mathcal{R}_m(x) = \sum_n (n+1) c_n \langle R_m^2 \rangle_n x^n \quad \propto \quad (1 - x/x_c)^{-(\gamma+2\nu+1)}, \quad (8)$$

$$\mathcal{R}_g(x) = \sum_n (n+1)^2 c_n \langle R_g^2 \rangle_n x^n \quad \propto \quad (1 - x/x_c)^{-(\gamma+2\nu+2)}, \quad (9)$$

where the factors under the sum ensure that the coefficients are integer valued. Here ν is another critical exponent with value $\nu = 3/4$ [5, 6].

Figure 3 displays results obtained from 3rd order differential approximants both un-biased ($q=0$) and biased with the order of the root at x_c being $q=2$ and 3, respectively. The left-most panels which are for the un-biased case again vividly illustrates that traditional differential approximants cannot quite reproduce the exact values of the critical exponents. As was the case for the SAW generating function the estimates from the mean-square end-to-end distance $\mathcal{R}_e(x)$ (top panel) and the mean-square monomer-to-end distance $\mathcal{R}_m(x)$ (middle panel) exhibit a slow systematic drift as N is increasing and ever so slowly they approach the exact value. The estimates from the mean-square radius-of-gyration $\mathcal{R}_g(x)$ (bottom panel) are particularly ‘poor’ and seem to settle at a value somewhat below the exact value. When we look at the $q = 2$ and 3 biased approximants we find a very good convergence of the estimates from $\mathcal{R}_e(x)$ and $\mathcal{R}_m(x)$ to the exact exponent values (note in particular the finer scale along the y -axis). For $\mathcal{R}_g(x)$ the estimates for large N are now clearly consistent with the exact value but the scatter among the exponent estimates is quite pronounced and much larger than for the other two series.

In table 3 we list estimates for the critical exponents of the three metric generating functions as obtained from the averaging procedure described above except in this case we use the approximants with $N \geq 63$. The data naturally confirm the qualitative

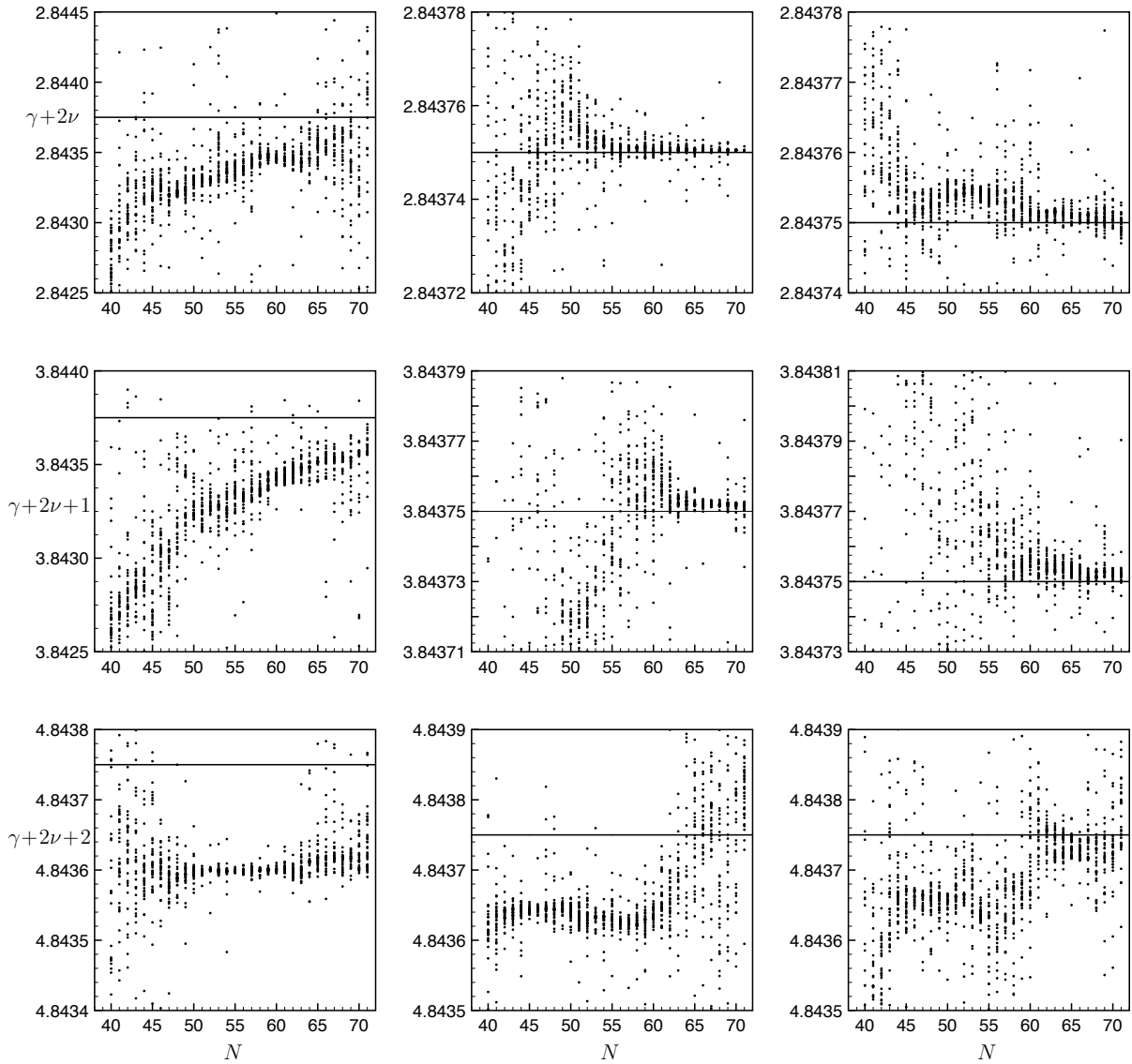


Figure 3. Estimates of the critical exponents for the metric properties of square lattice SAW. In each case the estimates are obtained from 3rd order differential approximants. From left to right are unbiased estimates and then biased estimates with $q = 2$ and 3 . From top to bottom are estimates to the generating function for the mean-square end-to-end distance, the mean-square monomer-to-end distance and the mean-square radius of gyration.

observations made from figure 3 but now in a quantitative manner. The estimates from un-biased approximants (column 2) are systematically lower than the exact value with ‘error-bounds’ that does not quite include the exact value. For the $q = 2$ and 3 cases the estimates for $\mathcal{R}_e(x)$ our estimate $\nu = 0.7500002(4)$ gives agreement with the exact exponent value $\nu = 3/4$ to 7 digits and thus provide a high accuracy confirmation of the exact value. The estimates for $\mathcal{R}_m(x)$ are generally an order of magnitude less accurate but again confirm the exact values. Finally, for $\mathcal{R}_g(x)$ we obtain estimates fully

Table 3. Estimates for the critical exponents of the generating functions for the mean-square end-to-end distance, mean-square monomer-to-end distance and mean square radius of gyration as obtained from K th order biased differential approximants.

Mean-square end-to-end distance					
$[K, q, r]$	$\gamma+2\nu$	$[K, q, r]$	$\gamma+2\nu$	$[K, q, r]$	$\gamma+2\nu$
$[2, 1, 0]$	2.843679(34)	$[2, 2, 0]$	2.84375113(29)		
$[3, 1, 0]$	2.843683(14)	$[3, 2, 0]$	2.84375050(14)	$[3, 3, 0]$	2.84375081(61)
$[4, 1, 0]$	2.8436984(58)	$[4, 2, 0]$	2.84375033(29)	$[4, 3, 0]$	2.84375064(24)

Mean-square monomer-to-end distance					
$[K, q, r]$	$\gamma+2\nu+1$	$[K, q, r]$	$\gamma+2\nu+1$	$[K, q, r]$	$\gamma+2\nu+1$
$[2, 1, 0]$	3.843649(31)	$[2, 2, 0]$	3.84375268(60)		
$[3, 1, 0]$	3.8436775(78)	$[3, 2, 0]$	3.84375198(47)	$[3, 3, 0]$	3.8437524(13)
$[4, 1, 0]$	3.8436803(72)	$[4, 2, 0]$	3.8437525(31)	$[4, 3, 0]$	3.8437524(14)

Mean-square radius of gyration					
$[K, q, r]$	$\gamma+2\nu+2$	$[K, q, r]$	$\gamma+2\nu+2$	$[K, q, r]$	$\gamma+2\nu+2$
$[2, 1, 0]$	4.8437055(82)	$[2, 2, 0]$	4.843691(64)		
$[3, 1, 0]$	4.8437183(92)	$[3, 2, 0]$	4.84375(10)	$[3, 3, 0]$	4.843734(24)
$[4, 1, 0]$	4.843714(17)	$[4, 2, 0]$	4.843673(76)	$[4, 3, 0]$	4.843743(66)

consistent with the exact value but now even less accurate. Curiously, the estimates for the un-biased case appear to be more accurate (as one can also confirm from figure 3), but this is quite clearly a ‘false’ convergence.

Finally we calculated biased estimates for the exponents γ_- at $-x_c$. Here we just quote results for $K = 3$ and 4 and $q = 2, r = 1$:

$$\mathcal{R}_e(x) \quad K = 3: \quad \gamma_- = 0.500027(63) \quad K = 4: \quad \gamma_- = 0.500050(42)$$

$$\mathcal{R}_m(x) \quad K = 3: \quad \gamma_- = -1.99952(11) \quad K = 4: \quad \gamma_- = -1.99952(16)$$

$$\mathcal{R}_g(x) \quad K = 3: \quad \gamma_- = -2.99965(13) \quad K = 4: \quad \gamma_- = -2.99968(40)$$

These estimates are clearly consistent with the exact values $\gamma_- = 1/2$ for $\mathcal{R}_e(x)$, $\gamma_- = -2$ for $\mathcal{R}_m(x)$ and $\gamma_- = -3$ for $\mathcal{R}_g(x)$.

4. Summary and Outlook

We made use of the fact that the critical point for square lattice self-avoiding walks is known very accurately to perform a numerical analysis of the SAW series using a new method for biased differential approximants. Our new method is a major advance since

it permits us to bias a differential approximant such that it has a singularity of order q (up to the order of the underlying differential equation). From the analysis with $q \geq 2$ we obtained exponent estimates in total agreement with the conjectured exact values $\gamma = 43/32$ and $\nu = 3/4$. In the case of the SAW generating function our conservative estimate $\gamma = 1.3437500(3)$ confirmed the exact value to at least 8 significant digits. This estimate is several orders of magnitude more accurate than the estimate from un-biased differential approximants and eliminates a long-standing minor discrepancy between exact and numerical results. In the case of the metric properties we obtain similar impressive estimates from the analysis of the mean-square end-to-end distance $\mathcal{R}_e(x)$ where our estimate $\nu = 0.7500002(4)$ confirmed the value of ν to 7 significant digits. The results for $\mathcal{R}_m(x)$ was not quite so impressive being an order of magnitude less accurate. The only slightly peculiar case was $\mathcal{R}_g(x)$ where the un-biased estimates appears to be quite accurate but wrongly gives an exponent estimate below the exact value while the biased estimates are consistent with the exact value but much less accurate. So in this case the biased exponents at least gives the correct answer which obviously is better than an accurate but wrong estimate. We also estimated the critical exponents γ_- at $-x_c$ and found exponent consistent with the exact values $\gamma_- = 1/2$ for SAW and $\mathcal{R}_e(x)$, $\gamma_- = -2$ for $\mathcal{R}_m(x)$ and $\gamma_- = -3$ for $\mathcal{R}_g(x)$. Finally, we tried to estimate the leading non-analytic correction-to-scaling exponent Δ from the biased exponent results when $q \geq 2$. We found results consistent with the exact conjectured value $\Delta = 3/2$ but somewhat disappointingly the estimates were not at all accurate.

The new method of biased differential approximants that we have introduced in this paper promises to be very useful in obtaining accurate exponent estimates in cases where the critical point(s) of a power-series is known exactly or very accurately. An obvious application is to various percolation series which have been notoriously difficult to analyse.

An interesting question is whether the method can be used to ‘reverse engineer’ more accurate estimates for critical points. In many cases (particularly 2D systems) critical exponents are known exactly but not so the critical points. Would it be possible to obtain improved estimates for the critical point say by calculating biased estimates for critical exponents while varying the biasing value of x_c . One might expect (or at least hope) that the biasing value of x_c yielding an exponent estimate equal to the exact value should be very close to the true critical point. A preliminary trial run using the square lattice SAP generating function confirmed the overall picture but did not give an improved estimate for x_c . But that is hardly surprising given that the un-biased estimates for x_c and α are already extremely accurate.

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